Appendix B

Source Code Tests

The source code for the numerical solution to Equation (2), incorporating reverse particle tracking, was tested against a number of benchmark cases for which the solution was exactly known. In addition, the simulations for these benchmark cases using reverse particle tracking were compared with simulations using the numerical schemes from two widely-applied water quality modeling packages, Water Quality for River-Reservoir Systems (WQRRS) (Smith, 1978) and QUAL2E (Brown and Barnwell, 1987).

NUMERICAL METHODS

Reverse Particle Tracking

Reverse particle tracking, the numerical method used in this study, is a mixed Eulerian-Lagrangian scheme. As described by Zhang et al (1993), the state variable is simulated in the advection step by sending a fictitious particle from each node, j (Figure 5), backward to the point,

$$x_j' = x_j - \int_{t_k}^{t_{k=1}} u^* \, dt \qquad \text{(B.1)}$$

where,

u^* = velocity encountered by the particle while moving from x'_j to x_j.

WQRRS

The numerical method used in WQRRS is a finite difference Eulerian scheme that begins with the mass balance equation for a state variable, T, stated in matrix form as

$$[V]\left\{\dot{T}\right\} = [S]\{T\} + \{P\} \qquad \text{(B.2)}$$

where,

[V] = matrix with element volumes on the diagonal and zeroes elsewhere,

$\left\{\dot{T}\right\}$ = vector of the rates of change of T in each element,

[S] = Matrix of coefficients multiplies the state variable, T,

{T} = Vector of the state variable in each segment,

[P] = Vector of constant terms for each segment.

Equation (B.2) is solved numerically by assuming

$$T_{t+\Delta t} = T_t + \frac{\Delta t}{2}(\dot{T}_t + \dot{T}_{t+\Delta t}) \qquad \text{(B.3)}$$

This leads to the following solution

$$\left[S^*\right]\left\{\dot{T}\right\} = \left\{P^*\right\} \qquad \text{(B.4)}$$

where,

$$\left[S^*\right] = [V] - \frac{\Delta t}{2}[S]$$

$$\left\{P^*\right\} = [S]\{B\} + \{P\}$$

$$B = T_t + \frac{\Delta t}{2}\dot{T}_t$$

<u>QUAL2E</u>

QUAL2E (Brown and Barnwell, 1987) uses an upstream, implicit method to solve the finite difference equation for a state variable, T

$$\frac{T_j^{k+1} - T_j^k}{\Delta t} = -\frac{Q_j\, T_j^{k+1} - Q_{j-1}\, T_{j-1}^{k+1}}{V_j} + r_j\, T_j^{k+1} + P_j \qquad \text{(B.5)}$$

where,

Q_j = flow out of the j^{th} element,

V_j = volume of the j^{th} element,

r_j = first order rate constant,

P_j = internal sources in the j^{th} element.

Equation (B.5) does not include a term for longitudinal dispersion, as does the more general form of the equation found in the QUAL2E documentation (Brown and Barnwell, 1987).

TEST CASES

Test Case A

Test Case A is based on an idealized river system 100 miles long divided into 100 equal segments. The longitudinal speed of the water is one mile/day. The boundary condition at x=0 for the state variable, T, is kept constant at 20 units and decays according to a first-order loss rate, K = 0.20. In a Lagrangian frame of reference

$$\frac{dT}{dt} = -KT \qquad (B.6)$$

And in Eulerian frame of reference

$$\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial x} = -KT \qquad (B.7)$$

where,

U = (constant) longitudinal speed of the water.

The solutions to Test Case A, obtained with reverse particle tracking, WQRRS and QUAL2E are shown in Figure B.1.

Test Case B

The geometry and hydrology for this case are the same as for Test Case A above. The boundary for the state variable, T, is varied according to

$$T(x=0) = 10 + 10\sin(2\pi t/P_0)$$

where,

P_0 = 10, 20, 50, 100 days

The results from the various numerical schemes are shown in Figures B.2 – B.5.

Test Case C

Test Case C uses the same geometry and hydrology as the previous two test cases. The boundary condition at X = 0 is defined as

$$T(t,x=0) = 20\ u_{-1}(t)$$

Where,

$u_{-1}(t)$ = the generalized function such that $T(t,x=0) = 0$ for $t<0$,

$T(t,x=0) = 1$ for $t>0$.

Results of simulations are shown in Figure B.6.

Test Case D

Test Case D is similar in all respects to Test Case B, with the exception that the segments used to describe the system are unequal and the periods associated with the harmonic functions describing the boundary conditions are

P_0 = 5, 10, 20, 50 days.

Segment 1 (the most upstream segment) is 0.5 miles in length, Segment 2 is 1.0 miles in length, Segment 3 is 1.5 miles in length, Segment 4 is 0.5 miles in length, Segment 5 is 1.0 miles in length, Segment 7 is 1.5 miles in length, the pattern repeating in this way for the entire length of the idealized system. The simulation results for this case are shown in Figures B.7 – B.10.

Test Case E

Test Case E is developed from solutions to the linearized form of the thermal energy budget equation (Edinger et al, 1974). In Lagrangian form,

$$\frac{dT}{dt} = K(T_{equil} - T) \qquad \text{(B.8)}$$

And in Eulerian form,

$$\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial x} = K(T_{equil} - T) \qquad \text{(B.9)}$$

where,

K = a first-order rate constant which is a function of meteorological parameters and water depth,

T_{equil} = water temperature at which there is no heat transfer across the the air-water interface,

= $T_{\Delta} \sin (2 \Pi t / P_{\Delta}) + T_{avg}$.

The Laplace transform gives the following solution

$$T(t) = T_0(t) + KT_{\Delta} \left[\frac{\cos(\omega(t-\tau))}{\omega^2 + K^2}(\omega e^{-K\tau} - \omega\cos(\omega\tau) + K\sin(\omega\tau))\right.$$

$$\left. + \frac{\sin(\omega(t-\tau)}{\omega^2 + K^2}(-K e^{-K\tau} + K\cos(\omega\tau) + \omega\sin(\omega\tau)\right] + T_{avg}(1 - e^{-K\tau}) \qquad \text{(B.10)}$$

where,

T_0 = boundary condition at $x = 0$

= $\Delta T_0 \sin (2 \Pi t / P_0) + T_{0\ avg}$,

ω = $2 \Pi / P_{\Delta}$,

τ = x/U.

Simulations were done for specific cases in which

ΔT_0 = 10,

$T_{0\ avg}$ = 10,

T_{Δ} = 10,

T_{avg} = 15,

P_{Δ} = 360,

P_0 = 5, 10, 20, 50,

x/U = 5.

The results are shown in Figures B.11 – B.14.

DISCUSSION

For the Test Case A, the steady-state problem with a first-order decay constant, K (Figure B.1), all three methods differ slightly from the exact solution. This error is a function of the ratio of the integration time step to the time constant (1/K). Reducing this ratio will also reduce the errors in all simulations.

Test Cases B – E provide indications of model performance in propagating high frequencies when advection is important. The reverse particle tracking method gives nearly exact solutions when the Courant number, $U \Delta x/\Delta t$, is equal to one (Test Cases, B, C, and E). For the case when the Courant number is not always equal to one (Test Case D), reverse particle begins to show the effects of numerical dispersion when the period, $P_0 = 10$ or lower.

Numerical dispersion is evident in simulations using WQRRS and QUAL2E for all test conditions including those where the Courant number is equal to one. In Test Cases B, C and D, the effects of numerical dispersion on amplitudes are severe when the period, $P_0 = 20$ or lower. WQRRS has somewhat better high-frequency response than QUAL2E, however. Both amplitude and phase of QUAL2E and WQRRS simulations are affected in Test Case E.